

A Review of Wave Packet Molecular Dynamics

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Abstract Warm dense matter systems created in the laboratory are highly dynamical. In such cases electron dynamics is often needed to accurately simulate the evolution and properties of the system. Large systems force one to make simple approximations enabling computational feasibility. Wave packet molecular dynamics (WPMD) provides a simple framework for simulating time-dependent quantum plasmas. Here, this method is reviewed. The different variants of WPMD are shown and compared and their validity is discussed.

1 Introduction

The creation of warm dense matter in the laboratory is a dynamic process. A large amount of energy is delivered to a target in a short period of time. Several different methods for delivering this energy have been developed, including exploding wire [1, 2, 3], laser foil [4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19], inertial confinement fusion [20, 21], ion beam [22, 23, 24, 25, 26, 27], Z machine [28, 29, 30, 31], free electron laser [32, 33, 34, 35], and laser induced shock [36, 37, 38, 39, 40, 41] experiments. Understanding energy exchange processes is crucial to the proper interpretation of these experiments. Lasers and ion beams deposit most of their energy in the electrons while shocks impart most of their energy to the ions. Energy absorption by the electrons in the former cases leads to a time-dependent light induced ionization and scattering [42, 43] or a stopping power problem [44, 45], respectively, while all of these cases produce electron-ion temperature relaxation [46]. Furthermore, electrons transport their energy via possibly non-equilibrium electrical and thermal conduction. Recent efforts [42, 43] to measure electron and ion dynamics at attosecond and picosecond timescales reinforce

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the need for a short-timescale simulation capability. It is now possible to directly image electron density [47] and such efforts can validate any theoretical predictions.

Ideally, one should calculate a numerically converged solution to the many-body time-dependent Schrödinger equation for the electron wave function in the external potential due to the time-dependent electron-ion interactions. Tens or a few hundred degrees of freedom can be evolved with the efficient multi-configuration time-dependent Hartree (MCTDH) method [48, 49]. Big simulations are needed to solve non-equilibrium systems for statistical reasons, to resolve gradients, and to resolve mean free paths of the particles in the system. Despite making significant progress in reducing computational effort for many-body quantum problems, MCTDH still scales exponentially with the number of degrees of freedom and cannot handle the system sizes needed for these systems. The obvious simplification would be to use time-dependent density functional theory [50] for which one would only need to evolve a three-dimensional density. However, very little is known about the accuracy of commonly used functionals for non-equilibrium high energy density systems. Finite computational resources then necessitate simple models that capture only the requisite quantum mechanics.

Wave packet molecular dynamics (WPMD) is a simple time-dependent quantum mechanical method with a rich underlying mathematical structure [51]. Here, WPMD is defined as the joint propagation of classical ions, represented as point particles, and quantum electrons, represented as wave packets. The wave packets are single electron states, localized in both position and momentum, and are combined via a Hartree product or Slater determinant to form the many-body wave function. Several groups have used WPMD to calculate a diverse set of observables, including equations of state [52, 53, 54, 55, 56, 57], the collision rate [58], electrical conductivity [54, 56], the diffusion coefficient [59], the dynamic structure factor [60], stopping power [61, 62], and shock Hugoniot curves [53, 55, 56, 63, 64]. In this chapter, the different derivations of the equations of motion for the wave packets are summarized in Sec. 2. The many different variations in wave packet forms used, antisymmetrization approximations, and interpretation of variational parameters are reviewed in Sec. 3 and an outlook is given in Sec. 4.

2 Theoretical Basis

2.1 Ehrenfest's Theorem

Quantum mechanics is infinitely more complicated than classical mechanics. Quantum dynamics happens within the full Hilbert space of the system while classical dynamics are described by a path through a finite-dimensional phase space. The quantum mechanical state does not correspond to any classical quantity such as position or momentum. We can, however, describe this state by its expectation values of moments of these quantities. Ehrenfest [65] was the first to show how these mo-

ments evolve with his famous theorem,

$$\frac{d}{dt} \langle \hat{A} \rangle = \frac{1}{i\hbar} \langle [\hat{A}, \hat{H}] \rangle + \left\langle \frac{\partial \hat{A}}{\partial t} \right\rangle, \quad (1)$$

where \hat{A} is an arbitrary operator and \hat{H} is the Hamiltonian operator, typically given by

$$\hat{H} = \sum_i \frac{\hat{p}_i^2}{2m_i} + \sum_{i<j} V_{ij}(\hat{\mathbf{r}}_i, \hat{\mathbf{r}}_j). \quad (2)$$

Here, the summations are over the particles in the system, V_{ij} is the interaction potential energy between particles i and j , and $\hat{\mathbf{p}}_i$, $\hat{\mathbf{r}}_i$, and m_i are the momentum operator, position operator, and mass of particle i , respectively. It is easy to show that

$$\frac{d}{dt} \langle \hat{\mathbf{r}}_i \rangle = \frac{\langle \hat{\mathbf{p}}_i \rangle}{m_i} \quad (3)$$

$$\frac{d}{dt} \langle \hat{\mathbf{p}}_i \rangle = - \sum_j \langle \nabla_i V_{ij} \rangle \quad (4)$$

$$\frac{d}{dt} \langle \hat{r}_i^2 \rangle = \frac{\langle \{ \hat{\mathbf{r}}_i, \hat{\mathbf{p}}_i \} \rangle}{m_i} \quad (5)$$

$$\frac{d}{dt} \langle \hat{p}_i^2 \rangle = \frac{1}{i\hbar} \sum_j \langle [\hat{p}_i^2, V_{ij}] \rangle, \quad (6)$$

where ∇_i is the gradient with respect to \mathbf{r}_i , the anti-commutator is defined as $\{ \hat{\mathbf{r}}_i, \hat{\mathbf{p}}_i \} = \hat{\mathbf{r}}_i \cdot \hat{\mathbf{p}}_i + \hat{\mathbf{p}}_i \cdot \hat{\mathbf{r}}_i$, and we have suppressed the dependence of V_{ij} on the position operators. These equations are only a few of the infinite number of equations needed to describe complete quantum dynamics. If V_{ij} is a smooth C^∞ function, then all of the time derivatives of $\langle \hat{\mathbf{r}}_i^n \hat{\mathbf{p}}_j^m \rangle$ for any i, j, n , and m will be a function of these same moments. So Ehrenfest's theorem leads to an infinite hierarchy of equations. These equations can be truncated at finite values of n and m with the help of a closure. For example, a common choice of restricted wave function in WPMD is the isotropic Gaussian for each quantum particle,

$$\varphi_G(\mathbf{r}_i) = \left(\frac{3}{2\pi\sigma^2} \right)^{3/4} \exp \left[- \left(\frac{3}{4\sigma^2} - \frac{ip_\sigma}{2\hbar\sigma} \right) |\mathbf{r} - \mathbf{r}_i|^2 + \frac{i\mathbf{p} \cdot (\mathbf{r} - \mathbf{r}_i)}{\hbar} \right], \quad (7)$$

where \mathbf{r}_i is the position coordinate, $\mathbf{r} = \langle \hat{\mathbf{r}}_i \rangle$ is its expectation value, $\mathbf{p} = \langle \hat{\mathbf{p}}_i \rangle$ is the expectation value of momentum, $\sigma = \sqrt{\langle \hat{r}_i^2 \rangle - |\langle \hat{\mathbf{r}}_i \rangle|^2}$ is the uncertainty in position, and p_σ is its conjugate momentum. Within the Hartree approximation, equations (3-6) imply

$$\dot{\mathbf{r}} = \frac{\mathbf{p}}{m_i} \quad (8)$$

$$\dot{\mathbf{p}} = - \sum_j \langle \nabla_i V_{ij} \rangle \quad (9)$$

$$\dot{\sigma} = \frac{p_\sigma}{m_i} \quad (10)$$

$$\dot{p}_\sigma = \frac{9\hbar^2}{4m_i\sigma^2} - \frac{1}{\sigma} \sum_j \langle (\hat{\mathbf{r}}_i - \mathbf{r}) \cdot \nabla_i V_{ij} \rangle. \quad (11)$$

These equations of motion predict that the center of the wave packet moves at the expectation value of velocity. This velocity changes according to the expectation value of the force. The width of the wave packet changes at a rate of p_σ/m_i , and its conjugate momentum evolves so as to satisfy the Heisenberg uncertainty principal and minimize the expectation value of the potential energy.

2.2 Local Harmonic Approximation

Heller's original formulation [66] of time-dependent semiclassical wave packet dynamics approached the problem differently. Instead of making a wave function ansatz, he expanded the potential energy to second order in the distance to the expectation value of the configuration of the system.

$$V(\mathbf{X}) \approx V(\tilde{\mathbf{X}}) + \nabla_{\mathbf{X}} V(\tilde{\mathbf{X}}) \cdot (\mathbf{X} - \tilde{\mathbf{X}}) + \frac{1}{2} \nabla_{\mathbf{X}} \otimes \nabla_{\mathbf{X}} V(\tilde{\mathbf{X}}) : (\mathbf{X} - \tilde{\mathbf{X}}) \otimes (\mathbf{X} - \tilde{\mathbf{X}}), \quad (12)$$

where $\mathbf{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$ is the set of positions of all N particles in the system, $\tilde{\mathbf{X}} = \langle \mathbf{X} \rangle$ is its expectation value, \otimes is the tensor product, and $:$ indicates the contraction of the indices of the rank-two tensors on either side of it. The system is then a $3N$ dimensional harmonic oscillator with characteristic frequencies that depend directly on $\tilde{\mathbf{X}}$ and so indirectly on time. The further simplification of neglecting the inter-particle terms in the last term of Eq. 12 and the particle statistics leads to an anisotropic formulation of WPMD. The potential energy has the reduced form:

$$V(\mathbf{X}) \approx \sum_i^N V_i(\tilde{\mathbf{x}}_i) + \nabla_{\mathbf{x}_i} V(\tilde{\mathbf{x}}_i) \cdot (\mathbf{x}_i - \tilde{\mathbf{x}}_i) + \frac{1}{2} \nabla_{\mathbf{x}_i} \otimes \nabla_{\mathbf{x}_i} V(\tilde{\mathbf{x}}_i) : (\mathbf{x}_i - \tilde{\mathbf{x}}_i) \otimes (\mathbf{x}_i - \tilde{\mathbf{x}}_i), \quad (13)$$

where $\tilde{\mathbf{x}}_i = \langle \mathbf{x}_i \rangle$, and the approximate many-body wave function is

$$\psi(\mathbf{X}, t) \approx \prod_i^N \left(\frac{\det \Sigma_i}{\pi} \right)^{1/4} e^{-\mathbf{(x}_i - \mathbf{r}_i)^T \cdot (\Sigma_i + i\Pi_i) \cdot (\mathbf{x}_i - \mathbf{r}_i) + i\mathbf{p}_i \cdot (\mathbf{x}_i - \mathbf{r}_i)/\hbar + i\xi_i}, \quad (14)$$

where Σ_i and Π_i , \mathbf{r}_i and \mathbf{p}_i , and ξ_i are time-dependent tensors, vectors, and scalars, respectively, which depend on the local value of potential energy and its derivatives. The main issue in applying this formulation to plasma physics is that the Coulomb potential is singular. So the expansion (12), is divergent near the singularities.

2.3 Time Dependent Variational Principle

One variational principle, proposed by McLachlan [67] and used in Refs. [59, 68], is to minimize

$$I(\psi, \theta) = \int |\dot{\psi} - \hat{H}\psi|^2 dV \quad (15)$$

with respect to $\theta = \partial\psi/\partial t$, where the integration is performed over all of configuration space.

The Dirac-Frenkel time-dependent variational principle (TDVP) [69] leads to a rigorous approximation of the time-dependent Schrödinger equation (TDSE) with a given variational ansatz. With this method the residual of the TDSE is minimized over a given subspace of states $|\psi\rangle$,

$$\delta \int_{t_i}^{t_f} \left\langle \psi \left| i\hbar \frac{\partial}{\partial t} - \hat{H} \right| \psi \right\rangle dt = 0, \quad (16)$$

where t_i and t_f are the initial and final times of the integration, and \hat{H} is the Hamiltonian. If the state $|\psi\rangle$ is allowed to vary throughout a Hilbert space that includes the solution, the TDSE will be exactly solved. Otherwise, the error in the state grows linearly with time over short times [70]. This variational principle is equivalent to the McLachlan approach for the most general form of a Gaussian wave packet [71].

A variational state $|\mathbf{q}\rangle$ can be parametrized by a vector of complex time-dependent variational parameters,

$$\mathbf{q} = \{q_1, q_2, \dots, q_{N_v}\}. \quad (17)$$

The variational parameters follow the equations of motion [70]:

$$i\mathbf{N}\dot{\mathbf{q}} = \frac{\partial \langle \hat{H} \rangle}{\partial \mathbf{q}^*}, \quad -i\mathbf{N}\dot{\mathbf{q}}^* = \frac{\partial \langle \hat{H} \rangle}{\partial \mathbf{q}}, \quad (18)$$

where $\langle \hat{H} \rangle = \langle \psi | \hat{H} | \psi \rangle$ and $*$ denotes the complex conjugate. The Hermitian norm matrix is defined by [70]:

$$N_{ab} = \frac{\partial}{\partial q_a^*} \frac{\partial}{\partial q_b} \ln \langle \mathbf{q} | \mathbf{q} \rangle. \quad (19)$$

Note, Eqs. (18) are time reversed forms of each other; so models derived from the TDVP preserve time reversal symmetry. For special choices of the variational form and parameters, the matrix \mathbf{N} reduces to a trivially-inverted matrix and canonical positions and momenta can be defined that make the equations of motion have a Hamilton form in N_v dimensions (see for example Ref. [72]):

$$\dot{\rho} = \frac{\partial \langle \hat{H} \rangle}{\partial \pi}, \quad \dot{\pi} = -\frac{\partial \langle \hat{H} \rangle}{\partial \rho}. \quad (20)$$

In spite of the persuasiveness of this form, it has to be noted that ρ and π are variational parameters inextricably tied to a particular variational wave function that should not be mistaken for classical positions and momenta if the quantum nature of the method is to be preserved. Using the TDVP with a small number of parameters requires physical intuition as to the form of the wave function. It must be flexible enough to give reasonable observables as well as numerically convenient and capable of representing the desired initial state.

3 Usage

3.1 Alternate Wave Packet Forms

The standard isotropic Gaussian form [Eq. (7)] for the wave packets in WPMD was mainly chosen for its mathematical simplicity. Expectation values of the kinetic energy and the potential energy for many different types of interactions (including the Coulomb potential) can be analytically calculated. This becomes a great utility in many-body dynamics, for which extensive calculations limit computationally-feasible system sizes. However, there is much to be desired physically from a variational form that this simple wave packet lacks. Well known asymptotic behaviors both near and far from nuclei are incorrectly modeled by Gaussians. The wave packets are unable to breakup and properly share their density with all the nuclei to produce an accurate representation of a free state, nor can an isotropic Gaussian accurately form bonds, but simple bonding can occur [57]. Furthermore, there is the issue of reconciling a periodic system with an aperiodic wave function. Various authors have made attempts to improve all of these shortcomings. Their trial wave functions are listed below:

- Anisotropic Gaussian [51]

$$\phi_{ag}(\mathbf{x}, t) = \left(\frac{\det \Sigma}{\pi} \right)^{1/4} e^{-(\mathbf{x}-\mathbf{r})^T \cdot (\Sigma + i\Pi) \cdot (\mathbf{x}-\mathbf{r}) + i\mathbf{p} \cdot (\mathbf{x}-\mathbf{r})/\hbar + i\xi}, \quad (21)$$

where Σ and Π are real symmetric matrices and Σ is positive definite. This form allows the Gaussians to evolve differently in each dimension. It is most useful for systems which have electron densities around each ion that are not isotropic, that is, when bonds are important.

- Hermite Gaussian Wave Packet [73]

$$\phi_{hg}(\mathbf{x}, t) = \sum_{i,j,k \in A} c_{ijk} \phi_{hg}^{ijk}(\mathbf{x}, t), \quad (22)$$

where the Hermite-Gauss functions ϕ_{hg}^{ijk} are

$$\varphi_{hg}^{ijk} = \prod_{j=x,y,z} h_{n_j}(\sqrt{\omega_j}(r_j - x_j)) \exp[-(\omega_j/2 + i\gamma_j)(r_j - x_j)^2 + ip_j(r_j - x_j)], \quad (23)$$

the h_{n_j} are the normalized Hermite polynomials of degree n_j , A is the set of allowed triplets, and ω_j , r_j , γ_j , and p_j are variational parameters. The set A can be restricted to reduce the numerical effort in inverting the overlap matrix; otherwise, in the limit that A includes all possible triplets, the Hermite Gaussian wave packet becomes exact for one-electron problems.

- Split Wave Packet [74, 75]

$$\varphi_s(\mathbf{x}, t) \propto \sum_{\alpha=1}^M c_{\alpha} \varphi_{\alpha}(\mathbf{x}, t), \quad (24)$$

where each wave packet (φ_{α}) has the same form as Eq. (7), and the variational parameters (\mathbf{r} , \mathbf{p} , σ , and p_{σ}) take on different values and evolve independently for each wave packet. This form represents a single electron wave function by M Gaussians with mixing coefficients c_{α} . It allows the wave packet to breakup, following the behavior observed in Ref. [75].

- Periodic Wave Packet [52, 53, 63]

$$\varphi_p(\mathbf{x}, t) \propto \sum_{\mathbf{n}} \varphi_G(\mathbf{x} - \mathbf{n}L), \quad (25)$$

where \mathbf{n} is a lattice index for the three-dimensional periodic system and L is the length of the periodic box. This form is more consistent with periodic boundary conditions used in bulk plasma simulations. It causes a large wave packet to be even more weakly interacting with the rest of the system and so be more likely to have divergent width.

- Periodic-Bloch Wave Packet [54, 56]

$$\varphi_{pb}(\mathbf{x}, t) = e^{i\mathbf{q}\cdot\mathbf{x}/\hbar} \varphi_p(\mathbf{x}), \quad (26)$$

where \mathbf{q} is the Bloch momentum.

- Bound-Free Wave Packets [76]

$$\varphi_b(\mathbf{x}, t) = \frac{1}{\sqrt{\pi a_0^3}} e^{-|\mathbf{x} - \mathbf{r}_I|/a_0}, \quad (27)$$

where a_0 is the Bohr radius and \mathbf{r}_I is the position of an ion,

$$\varphi_f(\mathbf{x}, t) = \left(\frac{3}{2\pi\sigma^2} \right)^{3/4} e^{3(\mathbf{x} - \mathbf{r})^2/4\sigma^2 + i\mathbf{p}\cdot(\mathbf{x} - \mathbf{r})/\hbar}, \quad (28)$$

and the width σ is fixed. Ebeling and Militzer used both of these forms to represent bound and free states. The electrons were allowed to transition between these states according to known cross sections. Of course, the exact bound and free states can differ significantly from φ_b and φ_f .

- Self Similar Wave Packet [77]

$$\varphi_{ss}(\mathbf{x}, t) = \sqrt{s^{-3} \rho_0 \left(\frac{\mathbf{x} - \mathbf{r}}{s} \right)} e^{i[\mathbf{p} \cdot (\mathbf{x} - \mathbf{r}) + p_s (\mathbf{x} - \mathbf{r})^2 / 2s] / \hbar + \phi}, \quad (29)$$

where s , \mathbf{r} , \mathbf{p} and p_s are time-dependent variational parameters and

$$\rho_0(\mathbf{x}) = \begin{cases} \left(\frac{1}{\pi G^2} \right)^{3/2} e^{-\mathbf{x}^2 / G^2} & \text{Gaussian} \\ \frac{1}{8\pi E} e^{-\mathbf{x} / E} & \text{Exponential} \end{cases} \quad (30)$$

Murillo and Timmermans compared the relative accuracy of the Gaussian and exponential forms of ρ_0 in calculating the ground state energies of hydrogenic systems, helium-like ions, and the hydrogen molecule. The exponential wave packet performed better for single atoms, but the Gaussian wave packet better reproduced the hydrogen molecular bond. It is unclear which is better for time dependent systems for which \mathbf{r} can become displaced from the positions of the ions or centers of bonds.

- Harmonically Constrained Wave Packet [78]

$$\varphi_h(\mathbf{x}, t) = \varphi_G(\mathbf{x}, t) e^{id(\mathbf{x} - \mathbf{r})^4 / \sigma^2}, \quad (31)$$

where d is an adjustable parameter which controls how large width σ can get. The consequences of fixing d are discussed in Sec. 3.2.

3.2 Width Constraints

It has been observed [52, 53, 58, 63, 78, 79, 80, 81] that at high enough temperatures that the mean width of the wave packets increases without bound unless the equations of motion are altered. A diverging width leads to a uniform electron density and diminished electron-ion and electron-electron interactions, preventing electron equilibration or the correct measurement of transport quantities.

The most common method of preventing width spreading was introduced in Ref. [79] and continued by Refs. [52, 53, 58, 63, 80, 81]. A harmonic constraint is added to the energy expectation value in an ad hoc fashion,

$$H_{Harm} = a\sigma^2, \quad (32)$$

where a is an adjustable parameter setting the mean width of the electrons. Alternatively, Ebeling and coworkers [78] were able to derive such an expression by changing the variational wave function to Eq. (31), giving a slightly different harmonic constraint,

$$H'_{Harm} = \frac{20d}{3m} \left(p_\sigma \sigma + \frac{14}{3} d \sigma^2 \right). \quad (33)$$

Changing the variational wave function to Eq. (31) strongly affects the properties of the wave function. To visualize the change, the Wigner density

$$f_W(\mathbf{R}, \mathbf{P}, t) = \frac{1}{(2\pi\hbar)^3} \int \varphi_h^*\left(\mathbf{R} + \frac{\mathbf{s}}{2}\right) \varphi_h\left(\mathbf{R} - \frac{\mathbf{s}}{2}\right) e^{i\mathbf{P}\cdot\mathbf{s}/\hbar} d^3s \quad (34)$$

was calculated at $\mathbf{R} = \{x, 0, 0\}$ and $\mathbf{P} = \{p_x, 0, 0\}$ for $\mathbf{r} = 0$, $\mathbf{p} = 0$, $p_\sigma = 0$, and $\sigma = 1 \text{ a.u.}$ for several different values of d and shown in Fig. 1. When $d \neq 0$ the Wigner density is twisted and develops a discontinuity in its derivatives near $x = 0$.

Morozov and Valuev [58] proposed two alternative constraints. They introduced periodic boundary conditions for the width coordinate (equivalent to a reflecting boundary condition at some maximum width). This change allowed the wave packets to equilibrate to a width distribution, but the equilibrated density was too constant. They also invented an energy-based constraint, in which the wave packets experienced a confining potential only if their interaction potential energy with the nearest ion were above a given threshold. By tuning this threshold they could obtain different results for the collision frequency. It is unlikely that every dynamical quantity will obtain the correct value at the same threshold energy.

The underlying assumption of the harmonic constraint is that a diverging wave packet width is unphysical. However, it is physical for wave packet widths to diverge, but they should localize near ions at the same time. In fact, the simplest system (a single electron wave packet in a vacuum) has a well known exact solution

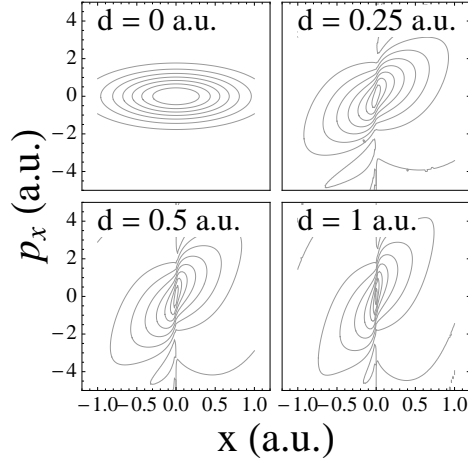


Fig. 1 Wigner density cross section of a three-dimensional Gaussian wave function with extra phase factor as in Eq. 31 for different values of d . The expectation values of position and momentum are zero, the width σ is one, and its conjugate momentum p_σ is zero.

which exhibits wave packet width divergence. Isocontours of the Wigner density are shown for the non-interacting wave packet in Fig. 2 at a series of different times. The time coordinate is defined so that the wave packets reaches a minimum uncertainty configuration at $t = 0$. At negative times the uncertainty in position is decreasing and at positive times it is increasing. The momentum uncertainty remains constant for this special case of the non-interacting wave packet because momentum eigenstates are also energy eigenstates. This behavior is generic to all non-interacting particles. At late times, they will always have a diverging width and will never reach minimum uncertainty again.

Grabowski *et al.* [75] showed that this divergence also occurs in their model plasma, made of a single dynamic electron propagating through a fixed periodic sys-

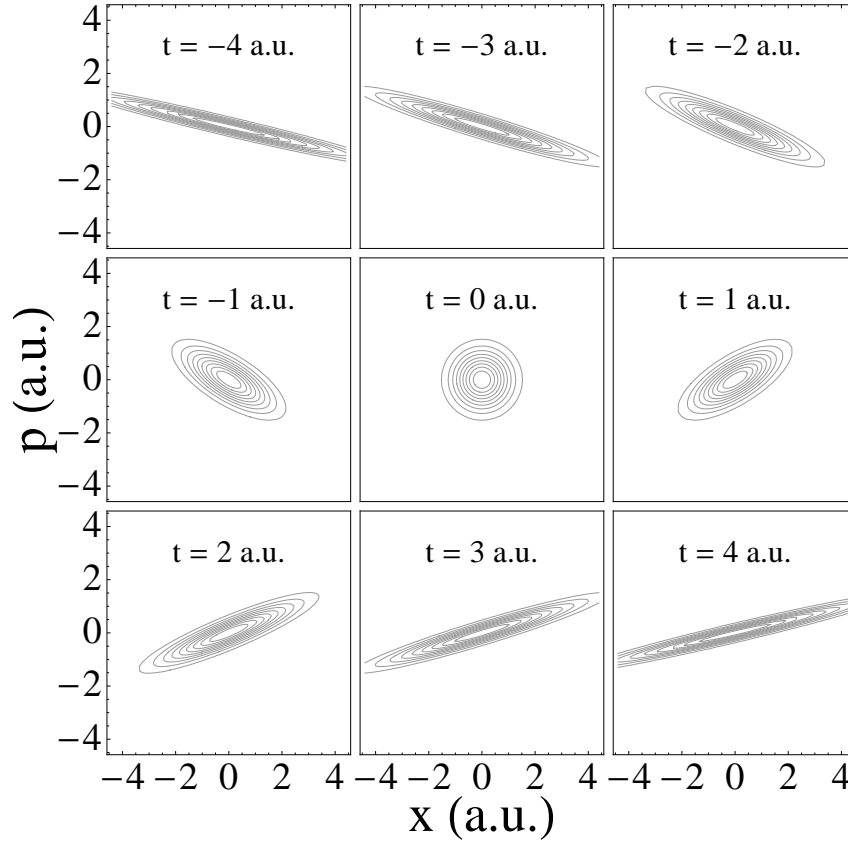


Fig. 2 Wigner density of a one-dimensional Gaussian wave function propagating in vacuum. The expectation values of position and momentum are zero at all times.

tem of statically screened protons. This simple system could be propagated exactly and it was observed that the simple wave packet variational form actually underestimates the spreading, and its main failure was its inability to individually scatter off each proton, which would have created the necessary fluctuations in density.

3.3 Antisymmetrization

The most computationally expensive part of a wave-function-based quantum calculation is the accurate treatment of Fermi statistics. Such a treatment requires a fully antisymmetrized many-body wave function, which becomes especially cumbersome when the single particle states are not orthogonal to each other as in WPMD. The totally antisymmetric wave function is

$$\psi(\mathbf{x}_1, \dots, \mathbf{x}_N, t) = n\hat{A} \prod_i \varphi_i(\mathbf{x}_i, t) \chi_i, \quad (35)$$

where $\{\mathbf{x}_1, \dots, \mathbf{x}_N\}$ are the coordinates of N electrons, t is time, χ_i is a Pauli spinor, n is a normalization constant, φ_i is i th wave packet, here of the form Eq. (7), \hat{A} is the antisymmetrization operator,

$$\hat{A} = \prod_{i < j} (1 - \hat{e}_{ij}), \quad (36)$$

and \hat{e}_{ij} is the exchange operator, which exchanges the positions and spins of particles i and j .

The expectation value of the Hamiltonian is needed to calculate the equations of motion of the variational parameters [see Eq. (18)]. The kinetic and potential expectation values for the state (35) are [70]

$$\langle \hat{T} \rangle = \sum_{k,l=1}^N \langle \varphi_k \chi_k | \hat{t} | \varphi_l \chi_l \rangle \mathcal{O}_{lk} \quad (37)$$

$$\langle \hat{V}_{ei} \rangle = \sum_{k,l=1}^N \langle \varphi_k \chi_k | \hat{v}_{ei} | \varphi_l \chi_l \rangle \mathcal{O}_{lk} \quad (38)$$

$$\langle \hat{V}_{ee} \rangle = \sum_{k,l,m,n=1}^N \langle \varphi_k \chi_k \varphi_l \chi_l | \hat{v}_{ee} | \varphi_m \chi_m \varphi_n \chi_n \rangle (\mathcal{O}_{mk} \mathcal{O}_{nl} - \mathcal{O}_{ml} \mathcal{O}_{nk}), \quad (39)$$

where \hat{t} is the single-body kinetic energy operator, \hat{v}_{ei} and \hat{v}_{ee} are the two-body electron-ion and electron-electron potential energy operators, respectively, and \mathcal{O}_{lk} is the inverse of the overlap matrix,

$$(\mathcal{O}^{-1})_{kl} = \langle \varphi_k \chi_k | \varphi_l \chi_l \rangle. \quad (40)$$

It is immediately apparent from Eq. (39) that one must complete an order N^4 operation per time step as well as deal with the possibility that the overlap matrix can become nearly singular, which explains why such calculations have mainly been limited to systems of finite size, such as the modeling of nucleons in a nucleus [70].

Using Eqs. (37) and (39), the energy and density of atoms can be calculated from the Raleigh-Ritz variational principle. The electron densities of the first six atoms on the periodic table are shown in Fig. 3 using individual electron wave packets of the form (7). Even with such a simple variational form, the correct shell structure is produced. Hydrogen has a single s orbital, helium has two s orbitals of the same size and opposite spin, lithium has two inner s orbitals and one outer, and beryllium has two inner and two outer s orbitals. The structure is more interesting for boron and carbon, in which pairs of wave packets are displaced on opposite sides of the nucleus in order to form effective p orbitals. So the boron electron density has a maximum along the z axis and a minimum in the x - y plane, while the carbon atom has maxima along the x and y axes and a minimum on the z axis. Of course, the detailed structure is wrong; the cusp condition is not satisfied and the density falls off too fast at infinity. However, having shell structure means antisymmetrized WPMD includes a simple version of bound-free transitions.

Due to the expense of full antisymmetrization, several different approximations have been made in the literature. The simplest approximation is the Hartree approximation,

$$\hat{A} \approx \hat{A}_1 = 1, \quad (41)$$

used in Refs. [58, 60, 78]. This approximation is valid at temperatures much above the Fermi energy. Unfortunately, this is also the regime in which wave packet

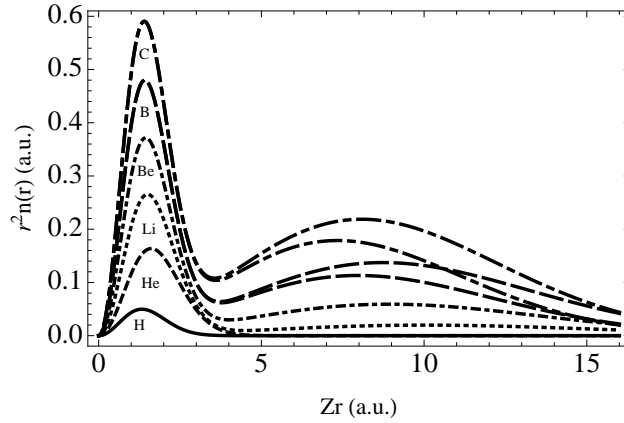


Fig. 3 Radial density of fully antisymmetrized variational wave functions for the lowest six elements of the periodic table: hydrogen (solid), helium (dashed), lithium (dotted), beryllium (dot-dashed), boron (long dashed), and carbon (long dot-dashed). Two curves are shown for boron and carbon to indicate anisotropy. These are the maximum and minimum densities found at each value of r .

spreading is the biggest issue, so width constraints were used in all of those references.

Klakow *et al.* [82, 83] published the first WPMD results for plasmas. They and others [79, 80, 84] used the pairwise antisymmetrization approximation

$$\hat{A} \approx \hat{A}_2 = 1 - \sum_{i < j} \hat{e}_{ij}, \quad (42)$$

which includes only two-body exchange. This approximation holds when all of the wave packets are well separated in phase space. That is, the distance between their expectation values of position and momentum is big compared to their uncertainties.

Another approximation [52, 53, 54, 56, 63] is to use the Hartree form while calculating the expectation value of the electron-electron potential energy, but use full antisymmetrization for the kinetic energy,

$$\langle V_{ee} \rangle \approx \sum_{k,l=1}^N \langle \varphi_k \chi_k \varphi_l \chi_l | \hat{v}_{ee} | \varphi_k \chi_k \varphi_l \chi_l \rangle. \quad (43)$$

Such a scheme allows simulations at temperatures up to 30,000K before wave packet divergence becomes an issue [58].

The simplest computational way of including exchange effects is through the empirical electron Force Field (eFF) model [55, 57, 64]. Energy expectation values are calculated with the Hartree approximation, but then corrected with a Pauli potential,

$$E_{Pauli} = \sum_{m_{s,i}=m_{s,j}} E(\uparrow\uparrow)_{ij} + \sum_{m_{s,i} \neq m_{s,j}} E(\uparrow\downarrow)_{ij}, \quad (44)$$

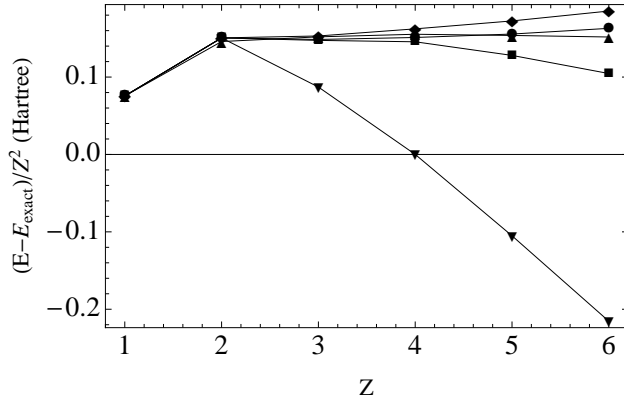


Fig. 4 Error in variational energy as a function of Z for different choices of approximation to the energy expectation value: Hartree (upside down triangles), antisymmetrized kinetic energy (squares), eFF (triangles), fully antisymmetrized (circles), and two-body exchange (diamonds).

$$E(\uparrow\uparrow)_{ij} = \left(\frac{S_{ij}^2}{1 - S_{ij}^2} + (1 - \rho) \frac{S_{ij}^2}{1 + S_{ij}^2} \right) \Delta T_{ij}, \quad (45)$$

$$E(\uparrow\uparrow)_{ij} = \frac{\rho S_{ij}^2}{1 + S_{ij}^2} \Delta T_{ij}, \quad (46)$$

$$\Delta T_{ij} = \frac{3}{2}(\bar{\sigma}_i^{-2} + \bar{\sigma}_j^{-2}) - \frac{2[3(\bar{\sigma}_i^2 + \bar{\sigma}_j^2) - 2\bar{r}_{ij}^2]}{(\bar{\sigma}_i^2 + \bar{\sigma}_j^2)^2}, \quad (47)$$

$$S_{ij} = \left(\frac{2}{\bar{\sigma}_i/\bar{\sigma}_j + \bar{\sigma}_j/\bar{\sigma}_i} \right)^{3/2} \exp \left(-\frac{\bar{r}_{ij}^2}{\bar{\sigma}_i^2 + \bar{\sigma}_j^2} \right), \quad (48)$$

where $\bar{\sigma}_i = c_1 \sigma_i$, $\bar{r}_{ij} = c_2 |\mathbf{r}_i - \mathbf{r}_j|$, and the empirical parameters $\rho = -0.2$, $c_1 = 0.9$ and $c_2 = 1.125$ are set by fitting to accurate molecular properties. The form of E_{Pauli} is motivated by terms which appear with two-body exchange.

Figure 4 shows the error in energy of the lowest six atoms on the periodic table using all of these antisymmetrization methods. Full antisymmetrization makes an error roughly equal to $0.15Z^2$ a.u. This error is due to the lack of inclusion of electron correlation and from the simple single electron variational form. Since the approximations made are with respect to the fully antisymmetrized Gaussian wave packet calculation, their accuracy should be determined by how close they are to that result. In order of accuracy, the approximations are eFF, two-body exchange, antisymmetrized kinetic energy, and the Hartree approximation.

3.4 Interpretation

The theoretical basis of WPMD is quantum mechanical. However, the variational parameters describing the electrons' wave function and the energy expectation value are often interpreted as if they are classical quantities. The latter quantity is continuous with a lower bound, necessarily greater than the true ground state due to the restriction of the Hilbert space to the subspace spanned by the Gaussian wave packets. There is confusion in the literature as to why this energy is not quantized for bound systems, which is taken to be a problem of the model [76]. However, intermediate energy expectation values can easily be reached by creating time-dependent states, which are mixtures of the states with the discrete energy eigenvalues, which is exactly the case here.

Another confusion arises with respect to the partition function. If the energy expectation value is taken to be classical and the width taken to be a classical fourth degree of freedom for each electron, then the classical partition function is divergent unless a width constraint is added. However, this is caused by the approximation

$$e^{-\beta \hat{H}} \approx e^{-\beta \langle \hat{H} \rangle}, \quad (49)$$

where β is the inverse temperature. In fact, exact thermodynamic properties can be calculated in any basis, including Gaussians. The interested reader is referred to Refs. [70] and [85] for accurate quantum treatments.

Within the plasma physics community dynamical quantities and transport coefficients have been calculated by interpreting the position and momentum expectation values as classical quantities and then using classical formulas [54, 56, 58, 60]. This choice along with the width constraints turns the WPMD model into an effective classical system meant to mimic properties of quantum mechanics; it is no longer an ab initio quantum model. Tuning this classical model to known quantities may still lead to sensical results.

4 Outlook

The dream of having a simple and accurate time-dependent method capable of accurately simulating WDM systems has not been fully realized. To model high temperature systems, of order or greater than the Fermi energy, either an unphysical width constraint must be used or the system develops an unphysical homogeneous density. At lower temperatures, the eFF variant of WPMD has made the greatest strides having been applied to such diverse calculations such as stopping power [57], equation of state [55], lithium cluster-slab impact [64], and the shock Hugoniot curves of liquid hydrogen and deuterium [55, 57, 64]. However, the empirical parameters in this model make it difficult to quantify errors a priori.

The greatest errors in WPMD stem from its simple variational form. Improvements for high temperature systems should focus on more accurate representations of delocalized free states that have higher densities near ions. The drive for a better representation of low temperature systems should focus on improving the ability of the wave packets to form bonds by allowing anisotropies.

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